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doi: 10.1103/PhysRevLett.55.1854

Langevin Simulation Including Dynamical Quark Loops

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(Received 9 April 1985)

A Langevin method is proposed for simulation of full QCD including dynamical quark loops. It is shown that the method works well once a proper discretization of the fictitious time is made. A realistic simulation with this method is perfectly feasible on vector computers presently available.

PACS numbers: 12.35.Cn, 02.50.+s, 02.70.+d, 11.15.Ha

Recent applications of Monte Carlo techniques to lattice gauge theories[1] have greatly facilitated our understanding of hadron dynamics. It has enabled us to calculate a variety of important physical quantities including, albeit within the quenched approximation, the hadron spectrum.[2] For a full treatment of lattice QCD, however, one needs efficient techniques for incorporating the effect of vacuum quark loops. The majority of the attempts so far utilized the pseudofermion technique.[3] More recently the microcanonical method[4] has been extended to include dynamical quarks.[5] Both methods involve approximations and assumptions which require a careful scrutiny for their justification: In the pseudofermion case, the ratio of the quark determinant is approximated by the leading term in the variation of the gauge variables. The validity of the microcanonical procedure hinges on the assumption of ergodicity besides the apparent drawback that the coupling constant has to be calculated through the simulation itself.

We point out that the Langevin formulation of field theories[6] provides an interesting alternative for solving full QCD including dynamical quark loops, which seems free from these potential sources of trouble. Inclusion of dynamical quark loops is achieved by expressing the quark determinant in terms of effective bosonic variables.[7] The solution of the corresponding Langevin equation generates an ensemble having the measure of full QCD. There is no approximation involved in the framework itself.

We have undertaken a study of the practical problems that arise in solving numerically the Langevin equation. Our study has revealed the following: (i) A conventional discretization of the fictitious time derivative leads to large systematic errors, especially for correlations at large distances, which practically invalidates the procedure. (ii) With a second-order improved discretization, however, the Langevin method works beautifully, both without and with dynamical quarks. Our extensive calculation with the SU(2) gauge group shows that the effect of quark loops substantially modifies the result obtained in the quenched approximation. A preliminary study for SU(3) indicates that a simulation on a 10^4 lattice or larger with several thousand sweeps is feasible with vector computers available today. We have also examined the microcanonical method. A comparison will be made with the Langevin method toward the end of this note.

We begin the consideration of systematic errors in the Langevin simulation for pure gauge system. Let $S(\mathbf{U})$ be the action with U_l the SU(N) gauge variable on the link l, and let $\nabla_l = t^a \nabla_l^a$ be the right derivative with $\nabla_l^a = \sum_{ij} (U_l t^a)_{ij} \partial/\partial U_{lij}$ and $\mathrm{tr}(t^a t^b) = \delta^{ab}$. The Langevin equation is given by[8]

$$-iU_l(\tau)^{-1}\frac{d}{d\tau}U_l(\tau) = -i\nabla_l S(\mathbf{U}(\tau)) + \eta_l(\tau), \tag{1}$$

with τ the fictitious time and $\eta_l(\tau) = t^a \eta_l^a(\tau)$ the Gaussian noise satisfying

$$\langle \eta_l^a(\tau)\eta_{l'}^b(\tau')\rangle = 2\delta_{ll'}\delta^{ab}\delta(\tau-\tau').$$

Let us discretize the time τ in steps of $\Delta\tau$ and write $U_l^{(n)} \equiv U_l(n\Delta\tau)$. The simplest discretization of (1) preserving the unitarity constraint on U_l is given by

$$U_l^{(n+1)} = U_l^{(n)} \exp\{iX_l(\mathbf{U}^{(n)}, \boldsymbol{\eta}^{(n)})\}, \tag{2a}$$

$$X_l(\mathbf{U}^{(n)}, \boldsymbol{\eta}^{(n)}) = -i\Delta\tau\nabla_l S(\mathbf{U}^{(n)}) + (\Delta\tau)^{1/2}\eta_l^{(n)}, \tag{2b}$$

and $\eta_l^{(n)} = t^a \eta_l^{a(n)}$ satisfies

$$\langle \eta_l^{a(n)}\eta_{l'}^{b(n')}\rangle = 2\delta_{ll'}\delta^{ab}\delta^{nn'}.$$

In Fig. 1, we show by open circles the SU(3) Wilson-loop averages for the standard single-plaquette action from the iterative solution of (2) with $\Delta\tau = 0.01$ on 4^4 lattice and compare them with the result of the Monte Carlo simulation (crosses). The Langevin result is systematically smaller and the difference between the two is substantial, especially for the 2×2 Wilson loop.

We found that this is a systematic error arising from

the discretization of time (2). To show this, we define the distribution function $\rho^{(n)}(\mathbf{U})$ by

$$\rho^{(n)}(\mathbf{U}) = \langle \textstyle\prod_l \delta(U_l; U_l^{(n)}) \rangle, \tag{3}$$

where $\langle \cdots \rangle$ denotes average over the noise $\eta^{(0)}, \ldots, \eta^{(n-1)}$. Substituting (2) and expanding in $\Delta\tau$, one finds that the Fokker-Planck equation for (2) takes the form

$$(1/\Delta\tau)(\rho^{(n+1)} - \rho^{(n)}) = -\mathscr{D}^{(n)}\rho^{(n)} - \Delta\tau \mathscr{D}_1^{(n)}\rho^{(n)} + O(\Delta\tau^2), \tag{4}$$

where the operators $D^{(n)}$ and $D_1^{(n)}$ are defined by

$$\mathscr{D}^{(n)}\rho^{(n)} \equiv \textstyle\sum_l \{\nabla_l^a(\nabla_l^a S^{(n)}\rho^{(n)}) + \nabla_l^a \nabla_l^a \rho^{(n)}\}, \tag{5}$$

$$\mathscr{D}_1^{(n)}\rho^{(n)} = -\sum_{l,l'} \{\tfrac{1}{2}\nabla_l^a \nabla_{l'}^b (\nabla_l^a S^{(n)} \nabla_{l'}^b S^{(n)} \rho^{(n)}) + \tfrac{1}{3}(\nabla_l^2 \nabla_{l'}^b + \nabla_{l'}^b \nabla_l^2 + \nabla_l^a \nabla_{l'}^b \nabla_l^a)(\nabla_{l'}^b S^{(n)} \rho^{(n)}) + \tfrac{1}{6}(\nabla_l^2 \nabla_{l'}^2 + \nabla_l^a \nabla_{l'}^2 \nabla_l^a + \nabla_l^a \nabla_{l'}^b \nabla_l^a \nabla_{l'}^b)\rho^{(n)}\}, \tag{6}$$

with $S^{(n)} \equiv S(\mathbf{U}^{(n)})$ and $\nabla_l^2 = \nabla_l^a \nabla_l^a$.

Equation (4) shows that the limiting distribution for the first-order discretization (2) deviates from the desired form $\exp(-S)$. The stationary solution ρ_∞ of (4) takes the form

$$\rho_\infty = \exp[-S - \Delta\tau \delta S_1 + O(\Delta\tau^2)], \tag{7a}$$

$$\delta S_1 = -\tfrac{1}{2}\textstyle\sum_l \nabla_l^2 S + \frac{1}{12} c_2 S + \frac{1}{4}\sum_l \nabla_l^a S \nabla_l^a S, \tag{7b}$$

where c_2 represents the quadratic Casimir invariant in the adjoint representation. For the standard single-plaquette action the first two terms of (7b) shift β to

$$\beta_{\text{eff}} = \{1 - [2(N^2-1)/N - \tfrac{1}{6}N]\Delta\tau\}\beta, \tag{8}$$

while the third term generates an additional action containing two plaquettes. Both these terms favor disordering of the gauge configuration. Hence we understand the trend in Fig. 1 that the Langevin result is smaller than the Monte Carlo value. The magnitude of the difference, estimated by ignoring the $(\nabla S)^2$ term for simplicity, is in rough accord with the data shown in Fig. 1.

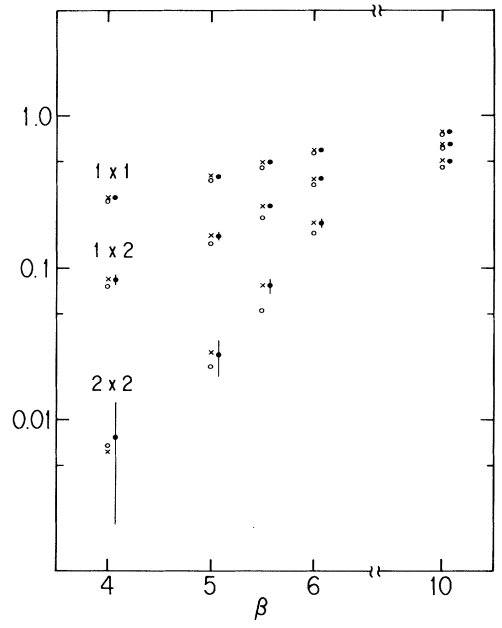

FIG. 1. Wilson loop for SU(3) pure gauge theory. Langevin results are represented by open and filled circles for naive and the second-order discretization, respectively. Crosses are Monte Carlo results. The error bars denote mean square deviation.

The systematic error could, in principle, be reduced by choosing $\Delta\tau$ sufficiently small. Unfortunately, 1% accuracy in $\beta_{\text{eff}}(\Delta\tau \lesssim 0.002)$ does not guarantee the same accuracy in the correlation functions because their β derivative is large at large distances, especially in the crossover region. Furthermore, the number of iterations needed to generate an independent configuration is proportional to $\Delta\tau^{-1}$, and hence so is the computer time. This makes the simulation including quarks practically impossible, for the computer time per iteration for full QCD is at least an order of magnitude more than that of the pure gauge case.

Clearly, reducing $\Delta\tau$ is not the way to diminish the systematic error. One rather needs an accurate discretization algorithm which ensures that the limiting distribution agrees with $\exp(-S)$ up to order $\Delta\tau$.[9] Our algorithm is given by

$$\begin{aligned} X_{0l}^{(n)} &= -i\Delta\tau \nabla_l S(\mathbf{U}^{(n)}) + (\Delta\tau)^{1/2}\eta_l^{(n)}, \\ U_l^{(n+1/2)} &= U_l^{(n)} \exp i X_{0l}^{(n)}, \\ X_{1l}^{(n)} &= -i\Delta\tau \nabla_l S(\mathbf{U}^{(n+1/2)}) + (\Delta\tau)^{1/2}\eta_l^{(n)}, \\ U_l^{(n+1)} &= U_l^{(n)} \exp\{i(\beta X_{0l}^{(n)} + \gamma X_{1l}^{(n)})\}. \end{aligned} \tag{9}$$

The requirement on the corresponding Fokker-Planck equation spelled out above is met if the parameters β

and γ satisfy

$$\beta=\tfrac{1}{2}+\Delta\tau\beta_1,\quad \gamma=\tfrac{1}{2}+\Delta\tau\gamma_1,$$
$$\beta_1+\gamma_1=\tfrac{1}{12}c_2, \tag{10}$$

and if the Gaussian noise $\eta_l^{(n)}=t^a\eta_l^{a(n)}$ is renormalized by

$$\langle\eta_l^{a(n)}\eta_{l'}^{b(n')}\rangle=2(1-\Delta\tau\tfrac{1}{4}c_2)\delta_{ll'}\delta^{ab}\delta^{nn'}. \tag{11}$$

In Fig. 1 we plot by filled circles the Wilson-loop averages from the second-order algorithm [(9)–(11)] with $\Delta\tau=0.01$ and $\beta_1=\gamma_1=c_2/24$. The very nice agreement with the Monte Carlo results demonstrates the effectiveness of this algorithm. With $\Delta\tau=0.01$, the systematic error is reduced by two orders of magnitude by repeating essentially twice the first-order algorithm and hence by using only twice the computer time. (We also carried out runs with $\Delta\tau$ up to 0.1. The systematic error exhibited a quadratic dependence for large $\Delta\tau$ as expected for the second-order algorithm. No noticeable deviation from the Monte Carlo values is found up to $\Delta\tau\sim 0.05$.)

We now describe the extension of the method to full QCD. The effect of vacuum quark loops arises from the determinant $\det D(\mathbf{U})$. If $D(\mathbf{U})$ is positive definite, $\det D(\mathbf{U})$ equals the Gaussian integral of a complex scalar field Y_s on site s with the action $S_f(\mathbf{U},\mathbf{Y})=Y_s^\dagger D^{-1}(\mathbf{U})_{ss'}Y_{s'}$. Thus, one may take

$$S_{\rm eff}(\mathbf{U},\mathbf{Y})=S_f(\mathbf{U},\mathbf{Y})+S(\mathbf{U}) \tag{12}$$

as the effective action for the full QCD.[7] The Langevin equation

$$-iU_l(\tau)^{-1}\frac{d}{d\tau}U_l(\tau)$$
$$=-i\nabla_l S_{\rm eff}(\mathbf{U}(\tau),\mathbf{Y}(\tau))+\eta_l(\tau), \tag{13}$$

$$\frac{d}{d\tau}Y_s(\tau)=-D^{-1}(\mathbf{U}(\tau))_{ss'}Y_{s'}(\tau)+\xi_s(\tau), \tag{14}$$

with η_l and ξ_s the Gaussian noise generates the distribution $\exp(-S_{\rm eff})$ as $\tau\to\infty$.[10]

In discretizing (13) and (14), a second-order algorithm is certainly needed to avoid systematic error. Using the Fokker-Planck equation, we found that the standard Runge-Kutta algorithm with $\langle\xi_s^{(n)}\xi_{s'}^{(n')\dagger}\rangle=2\delta_{ss'}\delta^{nn'}$ for (14), together with the discretization procedure [(9)–(11)] for (13) (with $S\to S_{\rm eff}$), gives the limiting distribution that deviates only by terms of $O(\Delta\tau^2)$ from $\exp(-S_{\rm eff})$. Compared with the pure gauge case, the additional complication is the calculation of $D^{-1}Y$ from Y which could be handled by standard methods such as conjugate gradient.

We have tested the above framework for SU(2) using Wilson's fermion action

$$D_0=1-K\{\textstyle\sum(1-\gamma_\mu)U_l+(1+\gamma_\mu)U_{l'}^\dagger$$

with two flavors ($D=D_0^\dagger D_0$). In Fig. 2(a) we show the K dependence of the Wilson loop and in 2(b) $\langle\bar\psi\psi\rangle$ at $\beta=4/g_0^2=2.0$ on a 4^4 lattice, the latter being calculated by the identity $\langle\bar\psi\psi\rangle=-\langle{\rm tr}(D^{-1}YY^\dagger D^{-1}\times D_0^\dagger)\rangle$. At each K, we carried out 2500 second-order iterations using the last 1500 iterations for the average ($\Delta\tau=0.01$).

The dynamical quark loops make the gauge configuration more ordered than in the pure gauge case. This is clearly visible in Fig. 2(a) beyond $K\sim 0.12$. (The points at $K=0$ are the Monte Carlo results for the pure gauge system.) The 4^4 lattice is probably too small to observe the effects of quark-pair creation in the static potential. It is nonetheless suggestive that the Wilson loop at $K\gtrsim 0.15$ plotted against area exhibits a concave shape in contrast to an exponential decrease for $K\gtrsim 0.12$. The loop effect is also apparent in the chiral order parameter [Fig. 2(b)] which deviates from the quenched value (cross) from $K\sim 0.12$.

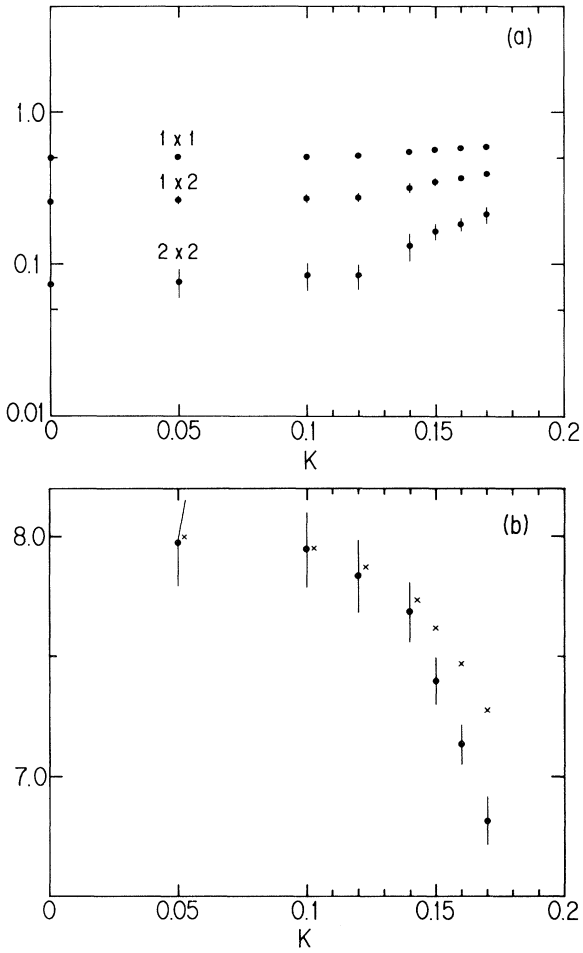

FIG. 2 (a) Wilson loop for full SU(2) theory with Wilson fermion (two flavors) at $\beta=2.0$ on 4^4 lattice. (b) $\langle\bar\psi\psi\rangle$ at $\beta=2.0$ on 4^4 lattice. Crosses represent the quenched value.

These trial results show that the effect of quark loops could be quite large so that the quenched results for properties of hadrons might be substantially modified.

A check on the systematic error is provided by the equality $\langle S_f \rangle = 4 \times 3 \times V$ with V the number of sites. The deviation of the measured value from this was less than 1%. We also repeated the calculation with a smaller time step, $\Delta\tau = 0.002$, and aside from the statistical fluctuation did not find any deviation from those of Fig. 2.

We examined the convergence by repeating the calculation with a different sequence of random numbers and a different type of initial configurations. The convergence was particularly slow around $K \sim 0.15$ compared with smaller or larger values of K. A plausible explanation is that at $K \sim 0.15$ the effective value of β reaches 2.2 at which a sharp crossover occurs in the pure gauge case.

The Langevin simulation is very much suited to vector computers. Our preliminary study shows that SU(3) simulation (Wilson fermion) on a 10^4 lattice can be done with about fifty megabytes of storage and about 30 h of computer time for 2500 iterations.

The microcanonical method[5] also tries to generate an ensemble governed by the effective action (12). In order to compare with the Langevin method, we have examined it for SU(2), paying particular attention to the questions associated with ergodicity.[11] We note that the ergodicity assumption fails in the limit of weak coupling and/or large quark mass since the system (or part of it) becomes integrable in these limits and hence by the Kolmogorov-Arnold-Moser theorem[12] invariant tori exist on the energy surface.

Our microcanonical formalism is slightly different from that of Ref. 5 in that $-U_l^{-1} dU_l/d\tau$ is identified with the gauge momentum and the gauge degree of freedom is fixed by the complete axial gauge. Our study on a 4^4 lattice shows that the method works for the pure gauge system; the Wilson loop averages agree with Monte Carlo values and the kinetic energy distribution coincides with that calculated from the microcanonical partition function. With quarks included, however, a delicate problem arises. On a 4^4 lattice (Wilson action) with $\Delta\tau = 0.01$, a large number of iterations $\sim (1\text{–}2) \times 10^4$ (to be compared with 2500 for the Langevin case) were necessary before the value of β obtained from the quark and gauge kinetic energies by the equipartition theorem agreed within a few percent. The situation was worse on a 2^4 lattice for which the two estimates of β in some runs differed by (10–20)% even after 2×10^4 iterations. This troublesome behavior was most prominent for β around 2.0 and for small K. While it is not quite clear if these results reflect some nonergodic behavior, it shows at least that the microcanonical method is less efficient than the Langevin in exploring the phase space of the system. Furthermore, though the values of Wilson loops and $\langle \bar{\psi}\psi \rangle$ obtained near $\beta \sim 2.0$ on a 4^4 lattice are consistent with those of the Langevin simulation, it is not clear to us how one could reliably estimate the error associated with the mismatch of β.

The Langevin method is apparently free from these problems of the microcanonical formalism, and we have shown above that it, indeed, works beautifully. We conclude by stressing that a realistic SU(3) simulation (on a 10^4 lattice or larger) with the Langevin algorithm presented in this note is prefectly feasible on presently available vector computers with regards to both storage and time consumption.

We are grateful to the Theory Division of The National Laboratory for High Energy Physics for warm hospitality and generous support for our work, to M. Okawa for informative discussions, and to Y. Oyanagi for advice on programming. One of us (A.U.) thanks Aspen Center for Physics for hospitality, where part of this work was done, and N. Christ, Y. Iwasaki, J. Kogut, O. Martin, and J. Polonyi for discussions.

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[9]One can develop a second-order discretization by modifying the X in (2b) with addition of terms of order $(\Delta\tau)$ [I. T. Drummond *et al.*, Nucl. Phys. **B200**, 119 (1983)]. The additional term, however, involves higher derivatives of the action of complicated form. Even worse, when quarks are included, this method requires an inversion of quark matrices $(D^{-1} \cdot \partial D/\partial U_l \cdot D^{-1} Y$, see text below for notation) for every link l on the lattice in each iteration, which is practically impossible [N. Christ, private communication].

[10]D. Zwanziger [Phys. Rev. Lett. **50**, 1886 (1983)] also proposed a Langevin method. Our method differs from his in one important aspect. His method uses $Y^\dagger DY$ for the effective quark action. In order to recover the correct distribution $(\det D)\exp(-S)$, this necessitates an extrapolation in the results whose magnitude seems difficult to bring under control, and hence should be avoided.

[11]M. Fukugita and A. Ukawa, to be published.

[12]See, for example, J. Moser, *Stable and Random Motions in Dynamical Systems* (Princeton Univ. Press, Princeton, N. J., 1973), and references therein.